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Compartmental Model Describing the Foliar Behavior of Tridiphane on Giant Foxtail

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A compartmental model of the foliar behavior of the postemergence grass herbicide tridiphane has been developed with use of data collected in an environmentally controlled ecosystem. Rate constants for penetration, desorption, volatility, and metabolism have been determined for the chemical applied to giant foxtail as a function of temperature, spray variables, and spray adjuvants. Temperature had the most dramatic effect on the rate constants, which increased 2–5-fold with each 10 °C rise in temperature. Crop oil concentrate (COC) adjuvant significantly increased the rate of foliar penetration with no effect on the volatility rate. Spray variables such as drop size and spray volume showed smaller effects. The model was tested under the varying environmental conditions in a field experiment and found to reasonably predict the behavior of tridiphane.

INTRODUCTION

Understanding the behavior of a pesticide following a foliar application is a complex problem. In the field a chemical is subjected to a variety of environmental conditions that affect the processes that act on the system: volatilization, penetration into the plant, metabolism, translocation. In addition, additives to the spray solution and spray variables (volume, droplet size, pressure) can affect the behavior of a chemical. Spray variables or wetting agents in the spray can affect distribution and coverage of the chemical on the plant, which may increase overall penetration of the chemical into the plant. Certain additives can directly increase penetration of chemicals through the cuticle of the leaf. These variables, plus the environmental effects on the rate processes, can enhance or restrict the net amount of chemical entering a plant and subsequently affect the biological efficacy of the material. Therefore, methods that attempt to quantitate the expected behavior of pesticides in plant systems can be useful in gaining insight into identifying the most important processes and application variables controlling chemical transport and transformations in plants.

Because of the variability encountered in the field, it is very difficult to conduct a well-controlled experiment to determine the effect of individual parameters on the foliar fate of a chemical. Therefore, a laboratory ecosystem has been designed after a system described by Nash and Beall (1977). This provides a standardized system for evaluation of chemical behavior in a controlled environment where environmental variables, formulation properties, and plant properties can be studied.

Compartmental computer models have been proposed to describe foliar uptake and movement of chemicals in plants (Bridges and Farrinton, 1974). Volatility of chemicals from plant surfaces has also been studied (Hartley, 1969; Nash et al., 1977). However, a realistic environmental model must consider collectively all the processes acting on the chemical. The modeling approach we have chosen is to describe as simply as possible the overall behavior of a chemical following a foliar application that will allow prediction of behavior in the field. We have not chosen at this stage to consider various plant substrate

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partitioning phenomena that could constitute more elaborate in-plant modeling such as that proposed by Price (1976).

Tridiphane [2-(2,2,2-trichloroethyl)-2-(3,5-dichlorophenyl)oxirane] is a new herbicide under development, recognized as exhibiting a synergistic relationship with atrazine [2-chloro-4-(ethylamino)-6-(isopropylamino)-*s*-triazine] with respect to selective weed control in corn when applied postemergently (Bugg and Witt, 1981; Zorner, 1983). Our research has focused on quantitating the relationships between tridiphane and atrazine in whole-plant systems. The work presented in this paper will discuss the development of modeling methods to better understand behavior of tridiphane when applied to giant foxtail.

MATERIALS AND METHODS

Environmental Chambers. The environmental chamber is an enclosed glass chamber located in a temperature-controlled room. It is designed for obtaining a mass balance of the chemical in the air, on the plant, and in the plant while studying its foliar behavior. Each chamber is constructed of 1-cm plate glass and measures 100 cm long, 50 cm wide, and 80 cm high. One side of the chamber has two sliding service panels to allow access to the inside of the chamber. Both ends of the chamber contain nine 5-cm holes for air inlet and outlet. They are centered 20 cm vertically and horizontally apart, with the bottom holes 30 cm above the bottom of the chamber. An air-outlet manifold encloses all nine air outlet holes to obtain equal suction through each hole. Each air outlet hole has a filter holder (10-cm i.d. × 7.5-cm length) cemented in front of the hole inside the chamber. These larger filter holders were a modification that was made from Nash's system to allow greater air flow.

Trapping filters consist of polyurethane foam, open-cell type, with a density of approximately 0.032 g/cm^3. Filters were cut 10 cm i.d. and 5-cm length. Air is drawn through the chamber and outlet filters with a $^1/_2$ HP high-pressure, direct-drive suction fan. Three chambers were connected through aluminum duct work with a damper to control air flow for each chamber. The duct work was then connected to the suction fan through flexible spring-steel reinforced hose. Under normal conditions the mean air flow through the chambers is approximately 0.8 km/h or 4 exchanges of air/min in the chambers. Air flow rates of 0.4 and 1.6 km/h were also studied in one experiment.

Located approximately 100 cm directly above each chamber is a 1000-W G.E. Duroglow Luminaire metal halide lamp. The lights were typically cycled with a 14-h photoperiod during the course of an experiment.

Tridiphane Formulations. Ring ^{14}C-labeled tridiphane was synthesized for use in these studies. Radiochemical assay by high-performance liquid chromatography (HPLC) showed the material to be 99% pure. Specific activity of the chemical was 14.0 mCi/mmol, and approximately 1.0 μCi was applied in 10 μL to a set of two plants for most experiments. Formulated tridiphane was made by weighing the desired amount of formulation blank (formulation with no tridiphane) into a conical 1-mL reaction vial, adding the appropriate amount of radiolabeled tridiphane dissolved in benzene, and removing the benzene under vacuum (50 mmHg). The resulting formulated material was then used in the experiments investigating foliar behavior. The formulation was made to simulate a 0.48 kg/L emulsifiable concentrate.

Application solutions were generally prepared to simulate spray solution concentrations and volumes that would be used in a field application. Since atrazine is commonly used in a tank mix with tridiphane, it was present in most of the experiments conducted. Solutions were prepared by diluting enough of the tridiphane formulation with water to give an application rate equivalent to 0.56 kg/ha in 280 L/ha. In the application volume study, dilution volumes of 90 and 180 L/ha were also used. In studies conducted in the presence of atrazine, atrazine was added to the application solution at a rate equivalent to 1.12 kg/ha using a 0.48 kg/L commercial atrazine formulation. All studies conducted with giant foxtail contained atrazine. Crop oil concentrate (COC), Atplus 411F, was used as an additive in many of the experiments generally at a rate equivalent to 2.3 L/ha. In the single study on the effects of COC, rates of 1.15 and 3.45 L/ha were investigated. A second oil (crop oil (CO), Sunspray 11E) was also studied in a separate experiment at 2.3, 4.6, and 6.9 L/ha rates. An example of the preparation of an application solution would be to dilute 1 μL of formulated tridiphane plus 2 μL of COC with 240 μL of water solution containing 2 μL of atrazine formulation.

Sample Treatment. Preliminary experiments to assess only the volatility of tridiphane were performed with glass slides in the chambers. Application solutions were prepared as described above, and studies were conducted with and without atrazine and COC at 20 and 30 °C. Twenty-five microliters of solution were applied in 0.5-μL drops to a glass slide, and the polyurethane foam plugs were exchanged periodically and analyzed for volatilized tridiphane. At the conclusion of each experiment, the glass slide was rinsed with 50 mL of methanol and analyzed for remaining tridiphane to determine the mass balance for the study.

Giant foxtail (*Setaria faberri*, L.) were grown in the greenhouse and used at the 2–3 leaf stage of growth. Plants were placed in the temperature-controlled room the night before beginning an experiment to acclimate them to the room conditions. Ten sets of plants, two plants per set, were treated with the application solution. Each plant would receive 5 μL of spray solution applied with a 25-μL syringe (10 drops/plant) in the standardized experimental situation. Plants were treated in the chambers with the air flow on to trap any chemical volatilized into the air. Plants were sampled at periodic intervals and analyzed for surface residues and absorbed chemical. The foam plugs were also changed at each sampling time and analyzed for trapped chemical.

Experiments were then conducted investigating the following variables: temperature, effects of the presence or absence of COC, air flow rate, application volume, amount of COC or CO as described above. A final experiment was conducted outside where the plant trays were set on a 1-m-high table, and the chemical was applied as described above.

Sample Analysis. Radioactivity trapped in the polyurethane foam plugs was extracted by rinsing each of the nine plugs three times with approximately 75 mL of acetone. The acetone extracts were combined to a final volume of 2000 mL, and 2 mL was counted (in duplicate) in 18 mL of Aquasol in a Packard 3255 liquid scintillation counter. The automatic external standard method was used to determine counting efficiency. The retention time on HPLC of the trapped material matched that of tridiphane and was assumed to be tridiphane.

Plants, cut at the soil surface, were first rinsed by dipping the plant in two successive 50-mL aliquots of methanol (5 s/rinse) to remove any chemical remaining on the plant surface. The plant and glass slide rinses were analyzed by liquid scintillation counting to quantitate the

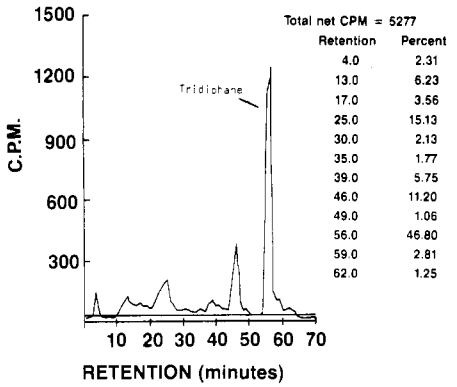

Figure 1. HPLC profile of radioactivity in 48-h plant extract where tridiphane + COC + atrazine was applied to giant foxtail at 20 °C (tridiphane retention time 56 min).

amount of radioactivity present and by HPLC to determine the nature of the residue. Liquid chromatography showed that only tridiphane was present in the leaf surface and glass slide rinses, indicating that no chemical reactions were taking place on these surfaces during the experiments.

The plants were then extracted with 10 mL of methanol in a polytron to release chemical that had penetrated the leaf. Radioactivity was again quantitated by counting 100 μL of the extract in 10 mL of Aquasol. The extracts were then analyzed for metabolites by HPLC. Typically, 200 μL of plant extract was injected on two Waters μBondapak C-18 columns connected in series. The sample was eluted with a water/methanol solvent system buffered at 0.01 M NH_4OAc at a flow rate of 1.5 mL/min. Following injection of the extract onto the column, 100% water was pumped for 3 min followed by a linear gradient run to 77% methanol at 25 min. This condition was held until 60 min when the system was programmed using a linear gradient to 100% methanol at 65 min. Tridiphane had an elution time of 56 min under these conditions.

Fractions of the column eluant were collected at 1-min intervals, diluted with 10 mL of Aquasol liquid scintillation cocktail, and counted in a Packard Model 3255 liquid scintillation counter. A profile of the radioactivity was reconstructed to determine the distribution of material in the extract. An example of a typical radioactivity elution profile is shown in Figure 1. For the development of the mathematical model, all non-tridiphane radioactivity was grouped together and called metabolites.

RESULTS AND DISCUSSION

Preliminary Experiments and Model Development. Initial work with tridiphane was conducted on glass slides. The rate of volatility was measured by using the tridiphane formulation with and without COC and atrazine at 20 and 30 °C. A plot of ln % tridiphane remaining vs. time is shown in Figure 2 for the 20 °C experiment without COC or atrazine. A straight-line relationship is obtained, indicating that first-order kinetics apply under the conditions of the test. The slope of the line is equal to the rate constant for volatilization. The results of all the glass slide experiments are summarized in Table I. Correlation coefficients shown in the table demonstrate the linearity of the data. It can be seen that addition of COC decreases the rate of volatility when present. This is presumably a result of solubilizing more of the tridiphane in the oil, which can act as a keeper. Atrazine, conversely, enhances volatility of the tridiphane slightly, possibly because of surface effects or because the atrazine is competing for the oil. As expected, an increase in temperature increases the rate of volatility significantly—approximately threefold from 20 to 30 °C.

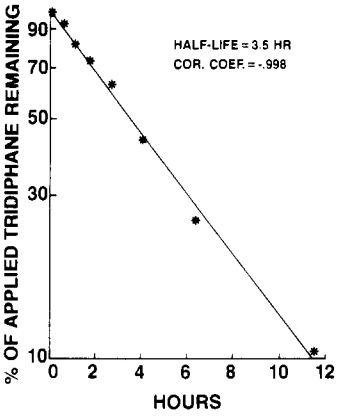

Figure 2. Tridiphane volatility from glass surface.

Table I. Volatility of Tridiphane from a Glass Surface with or without COC and Atrazine

treatment	temp, °C	k_v, h^{-1}	half-life, h	correln coeff (r)	rec, %
tridiphane	20	0.200	3.5	0.998	96.8
tridiphane + COC	20	0.060	11.5	0.999	99.4
tridiphane + COC + atrazine	20	0.100	7.0	0.999	98.6
tridiphane + COC	30	0.178	3.9	0.999	96.0
tridiphane + COC + atrazine	30	0.240	2.9	0.998	97.1

Also shown in Table I are the recovery data for these experiments using glass slides. As can be seen, the recoveries are, on the average, greater than 97%. Considering that several changes of the plugs were made throughout these experiments, these recoveries indicate that essentially all of the volatilized tridiphane is trapped by the plugs and that the chambers provide a convenient means to obtain a mass balance of this foliar system.

Following the work on glass slides, the behavior of tridiphane was studied on giant foxtail. The following model (eq 1) was shown to most adequately describe the behavior

$$C_{ar} \xleftarrow{k_v} C_{sf} \underset{k_d}{\overset{k_a}{\rightleftharpoons}} C_{ps} \xrightarrow{k_{ms}} C_{ms} \quad (1)$$

of tridiphane applied to giant foxtail as described in Material and Methods, where C_{ar} = amount of chemical in the air, C_{sf} = amount of chemical on the plant surface, C_{ps} = amount of chemical in the plant, C_{ms} = plant-soluble metabolites, k_v = rate constant for volatility, k_a = rate constant for absorption into plant, k_d = rate constant for desorption from plant, and k_{ms} = rate constant for metabolite formation.

The following set of differential equations (eq 2–5) was solved numerically on the IBM 370 using Dow Advanced Continuous Simulation Language (DACSL). The data were fit by using a relative least-squares optimization routine to determine the rate constants for each data set.

$$dC_{ar}/dt = k_v C_{sf} \quad (2)$$

$$dC_{sf}/dt = -(k_v + k_a)C_{sf} + k_d C_{ps} \quad (3)$$

$$dC_{ps}/dt = -(k_d + k_{ms})C_{ps} + k_a C_{sf} \quad (4)$$

$$dC_{ms}/dt = k_{ms} C_{ps} \quad (5)$$

All processes were considered to be first order with respect to the transfer of chemical between compartments. The reversible desorption process regulated by rate constant k_d was required to account for movement of the

Table II. Foliar Model Rate of Constants for Tridiphane + Atrazine (+, -) (2.3 L/ha of COC) at 12, 20, and 30 °C

temp, °C	COC	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}	k_{ms}, h^{-1}
12	+	0.053 ± 0.03[a]	0.148 ± 0.02	0.038 ± 0.003	
12	-	0.059 ± 0.006	0.033 ± 0.006	0.003 ± 0.001	
20	+	0.179 ± 0.04	0.335 ± 0.05	0.102 ± 0.02	0.010 ± 0.006
20	-	0.178 ± 0.02	0.111 ± 0.03	0.028 ± 0.005	0.010 ± 0.009
30	+	0.511 ± 0.02	1.070 ± 0.04	0.396 ± 0.07	0.012 ± 0.005
30	-	0.576 ± 0.02	0.575 ± 0.01	0.140 ± 0.02	0.012 ± 0.002

[a] 95% confidence interval.

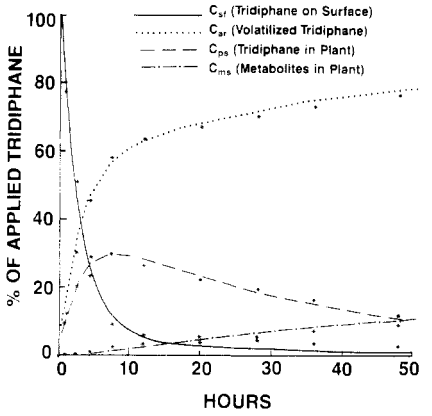

Figure 3. Distribution of tridiphane in various foliar compartments with time following application of tridiphane + atrazine without COC at 20 °C.

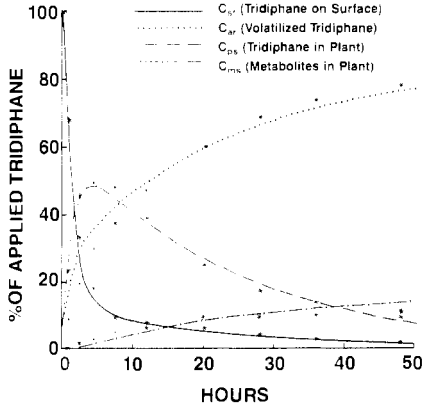

Figure 4. Distribution of tridiphane in various foliar compartments with time following application of tridiphane + atrazine with COC at 20 °C.

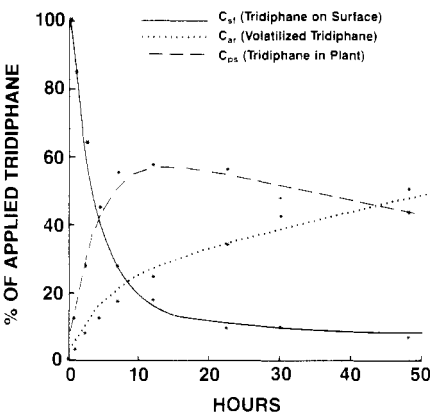

Figure 5. Distribution of tridiphane in various foliar compartments with time following application of tridiphane + atrazine with COC at 12 °C.

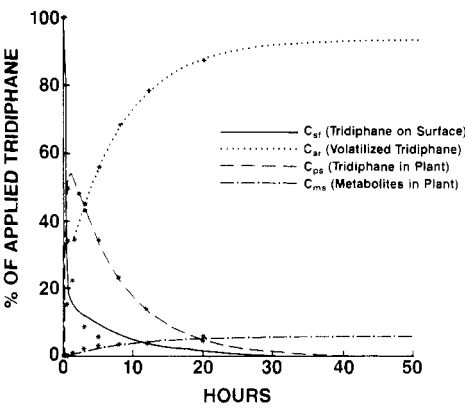

Figure 6. Distribution of tridiphane in various foliar compartments with time following application of tridiphane + atrazine with COC at 30 °C.

chemical back to the surface and into the air after the surface concentration approached zero. Apparently, immediately following application to the leaf a concentration gradient exists across the cuticle into the subcuticular region of the leaf. However, after the surface concentration is depleted through penetration and volatility, the direction of the gradient changes, allowing the chemical to be transported back across the cuticle before the chemical moves further into the plant or is metabolized.

As mentioned earlier, we attempted to find the simplest model to fit the data. Clearly a more sophisticated model may provide a better fit. However, this system of data analysis enabled us to make quantitative comparisons between experiments to evaluate the behavior of tridiphane under different environmental and application conditions.

Examples of the fit of the model to the compartmental values of tridiphane at 20 °C with and without COC are shown in Figures 3 and 4. Rate constants for these data are given in Table II. Examination of plots show that when COC is absent, the data points fall very close to the curves generated by the model. In the presence of COC, slightly more variation in the fit is observed; however, the overall behavior of tridiphane is adequately described by the model. Variation in the rate constants at the 95% confidence interval is shown with the data. In general, the calculated error is small, demonstrating the goodness of fit of the model to the data.

Temperature Experiments. The behavior of tridiphane on giant foxtail was investigated at 12, 20, and 30 °C. Experiments were conducted at rates of application equivalent to 0.56 kg/ha of tridiphane and 1.12 kg/ha of atrazine and in the presence and absence of 2.3 L/ha of COC. The data for the 12 and 30 °C experiments with COC are plotted in Figures 5 and 6. These data show the dramatic effect temperature has on the behavior of the chemical over the first 48 h following application. The experiments conducted without COC at 20 and 30 °C showed similar decreases in the amount of tridiphane penetrating the leaf as in the 20 °C data without COC shown in Figure 3. The rate constants for each experiment are given in Table II. It can be seen that for each increment in temperature the rate constants approximately triple. It can also be noted that the COC has little effect

Table III. Effects of System Variables on Foliar Model Rate Constants

Air Flow Study			
air flow, km/h	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}
0.4	0.15 ± 0.03[a]	0.32 ± 0.05	0.11 ± 0.07
0.8	0.15 ± 0.03	0.38 ± 0.03	0.15 ± 0.08
1.6	0.19 ± 0.03	0.30 ± 0.04	0.10 ± 0.07
COC Study			
COC, L/ha	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}
1.15	0.16 ± 0.03	0.39 ± 0.05	0.07 ± 0.07
2.3	0.19 ± 0.06	0.32 ± 0.10	0.09 ± 0.13
4.6	0.14 ± 0.02	0.36 ± 0.03	0.12 ± 0.05
Drop Size Study			
drop size, μm	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}
600	0.18 ± 0.02	0.52 ± 0.10	0.13 ± 0.06
800	0.15 ± 0.03	0.38 ± 0.03	0.13 ± 0.07
1000	0.17 ± 0.04	0.49 ± 0.06	0.13 ± 0.07
Spray Volume Study			
spray vol, L/ha	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}
90	0.09 ± 0.05	0.26 ± 0.02	0.11 ± 0.07
180	0.11 ± 0.04	0.35 ± 0.03	0.14 ± 0.07
280	0.16 ± 0.03	0.43 ± 0.03	0.13 ± 0.05
CO Study			
CO, L/ha	k_v, h^{-1}	k_a, h^{-1}	k_d, h^{-1}
2.3	0.16 ± 0.02	0.39 ± 0.05	0.07 ± 0.02
4.6	0.12 ± 0.05	0.32 ± 0.05	0.09 ± 0.06
6.9	0.12 ± 0.03	0.36 ± 0.07	0.12 ± 0.08

[a] 95% confidence interval.

on the volatility rate constant (k_v) unlike the results of the glass slide experiments. The volatility rate constant is very similar to that on the glass slide with tridiphane alone. The COC does, however, have a dramatic effect on the absorption and desorption rate constants. The absorption rate constant, k_a, increases 5×, 3×, and 2× at 12, 20, and 30 °C, respectively, while k_d increases 10×, 5×, and 3× at these temperatures in the presence of COC. Therefore, it appears that the COC enhances penetration of tridiphane into the plant, and while it also enhances desorption from the plant, the overall effect is that more chemical gets into the plant.

Considering the interaction of the chemical with the plant surface, where movement was observed in both directions across the cuticle, the question was raised as to where the chemical was in the plant: in the waxy layer of the cuticle, in the pectinaceous layer below the cuticle, or inside the plant cells below the pectinaceous layer. The possibility of the chemical being associated with the wax was investigated by washing treated plants with methylene chloride (which will remove the wax) at times when peak levels of tridiphane were in the plant. Very little material was removed with this wash, indicating the chemical is at least below this layer. Differentiation between the other possibilities mentioned is difficult and was not pursued further.

Effects of Other System Parameters on Rate Constants. To determine how other system variables might affect the foliar behavior of tridiphane, several experiments were conducted to investigate the rate of air flow, spray droplet size, spray volume, COC concentration, and CO (Sunspray 11E) concentration in individual experiments. The results of these studies are summarized in terms of the volatility, absorption, and desorption rate constants in Table III. All studies were conducted at 20 °C.

In the air flow experiment three different rates of air movement through the chambers were tested. The data in Table III show that little change was observed in the model rate constants. This result suggests that the rate-limiting process for volatility is diffusion of the chemical from the leaf surface. Once the chemical has diffused away from the plant surface, it is carried away by the air; however, the amount of air passing across the plant had little effect on the process.

Two studies were conducted investigating the effects of the addition of oils to the spray solution. In our earlier work a dramatic effect on the absorption of tridiphane was observed when COC was present. In the first experiment here, various levels of COC were studied: 1.15, 2.3, and 3.45 L/ha. Essentially no differences in the rate constants were detected at the levels of COC studied. In the second study crop oil (CO), Sunspray 11E, was studied at three levels of 2.3, 4.6, and 6.9 L/ha. Again, no significant differences in tridiphane behavior were observed at the different rates of CO or between CO and COC. Therefore, it appears that the presence of oil enhances absorption of tridiphane, and in general the lower concentrations appear to affect the absorption/desorption processes the same as the higher ones studied. However, the oil is generally employed in the application to increase atrazine penetration, and the effects of these various levels of oils on atrazine penetration behavior may be important but is not known at this time.

In the drop size study, three different drop sizes were studied to see whether tridiphane behavior was dependent on size or number of drops on the leaf. Over the range of sizes studied, no effects on the rate constants were observed. In the experiments drops are applied by syringe to control the application of the radioactive material, and the drop sizes used are at the large end of normally encountered drop sizes in a field application. Therefore, the conditions are not totally representative of field conditions; however, if drop size significantly affected plant penetration, we would have expected to see some effect in these studies.

In the final study of this type summarized in Table III, spray volume was investigated by applying the tridiphane formulation in 90, 180, and 280 L/ha application volumes. Therefore, each treatment received the same amount of chemical; however, in the lower application volumes fewer drops of higher concentration were applied. There were slight differences observed in this study compared to the previous studies. Each of these experiments was run side by side; however, conditions may have varied slightly from one test to the next. Therefore, some variation in the rate constants is observed between tests although small. In the spray volume study there were significant differences within the test. At lower spray volumes the volatility rate constant was lower; however, the rate of absorption was also lower such that there were not great differences in the overall behavior of the chemical. Theoretically, if a thicker layer of chemical is deposited in a lower spray volume application, the thickness of the layer could affect both the rate of volatility and absorption, reducing both these rates as the layer becomes thicker.

The reproducibility of the experimental procedures can be evaluated by examination of the rate constants in Tables II and III obtained under the standard condition of 0.56 kg/ha of tridiphane applied in a 280 L/ha application volume at 20 °C with 2.3 L/ha of COC and an air flow of 0.8 km/h. This condition is repeated five times throughout the studies conducted, with good agreement of the rate constants each time the study was repeated. This type of reproducibility is mainly accomplished through temperature control; without it comparisons of different application

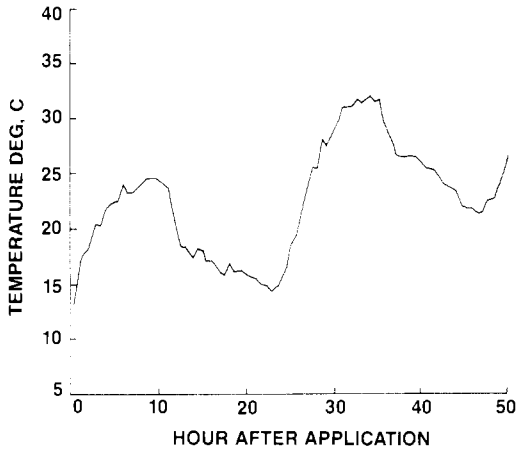

Figure 7. Temperature profile during the course of the outdoor experiments with tridiphane.

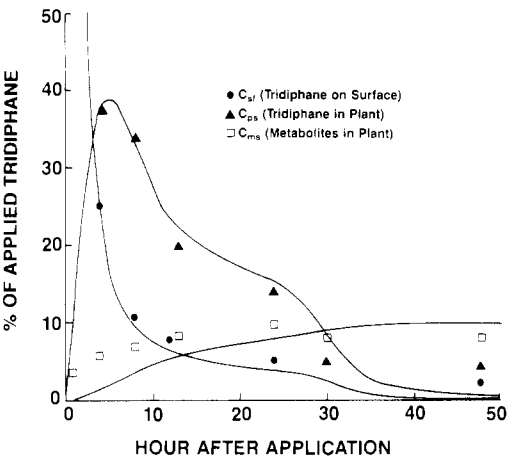

Figure 8. Distribution of tridiphane in various foliar compartments in outdoor experiment.

techniques and development of the model would not be possible.

Field Experiment. Giant foxtail plants were grown outside and treated with tridiphane, and the behavior of the chemical was followed for 2 days to test the model under field conditions. The plants were treated as in the laboratory studies with 0.56 kg/ha of tridiphane, 1.12 kg/ha of atrazine, and 2.3 L/ha of COC in the equivalent of 280 L/ha application solution. The temperature was monitored at 30-min intervals over the course of the experiment with a temperature probe set in with the plants. A plot of the temperature profile is shown in Figure 7. Temperature at the time of application was 12 °C, and daily highs were 25 and 32 °C for the successive days of the study. Air monitoring for tridiphane was not conducted in the field. The difference between radioactivity recovered on the plant surface and in the plant from that applied was assumed to have volatilized into the air.

To account for changes in the rate constants with temperature, the relationships (eq 6–9) were developed from the laboratory-measured rate constants in the temperature studies where T = the temperature (°C).

$$k_v = 0.015e^{0.125T} \quad (6)$$

$$k_a = 0.038e^{0.110T} \quad (7)$$

$$k_d = 0.0082e^{0.131T} \quad (8)$$

$$k_{ms} = 0.0080T - 0.00243 \quad (9)$$

With the exception of k_{ms}, the dependence of the rate constants on temperature fits the exponential relationships shown. The metabolic rate constant, which was only measured at 20 and 30 °C, was assumed to be a linear relationship. These relationships were used with the equations for the model and the temperature data to generate predicted levels of tridiphane in each compartment. The initial prediction based on the level of chemical in the plant overestimated the levels by approximately 10%, and the other compartments were slightly underestimated. The shape of the curve essentially paralleled the data, so the coefficient of the absorption expression was lowered to 0.030 to decrease the rate of absorption. The change in the apparent rate of absorption into the plant could be a result of a thicker cuticle being present in a outdoor-grown plant resulting in slower penetration of the chemical. The fit of the compartmental data with this change is shown in Figure 8. With this minor adjustment to the temperature relationships, a reasonably good fit of the data was obtained. The amount of tridiphane on the surface of the plants and in the plant corresponded very closely with the predicted estimates for these compartments. The fit of the metabolite pattern was not as good, in particular at earlier times. The level of metabolites rose more quickly than expected from the laboratory data. This could have been a result of faster metabolism in the field-grown plants or possibly the formation of impurities in our application solution. Overall, the approximate level of metabolite production after 2 days was close to the estimated value.

This test of the model demonstrates that tools such as the environmental chambers and modeling techniques discussed in this paper can be very useful in understanding the behavior of chemicals when applied in a foliar environment. Methods like this quantitate expected behavior based upon physical and biological relationships and can provide insight into understanding the environmental fate of a foliar-applied pesticide, the mode of transport and mechanisms of metabolism in the plants, formulation development, and the effects of spray variables on chemical behavior.

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